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Melting point–solubility–structure correlations in chiral and racemic model cocrystals

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Abstract

The impact of chirality is assessed via comparison of structural features and properties of binary cocrystals. 4,4'-Bipyridine and 1,2-bis(4-pyridyl)ethane were combined with achiral, racemic mixture or pure enantiomers of selected carboxylic acids with similar constituents (p-toluic acid, rac-2-phenylbutyric acid, racemic or S-phenylsuccinic acid). Single crystal structures, thermal analysis, powder X-ray analysis and equilibrium solubility in water and ethanol of the cocrystals were measured. It was concluded that the aqueous solubility of the cocrystals is inversely related to their melting points and this trend can be linked to some packing features. It was shown that the introduction of a chiral building block limits the formation of certain intermolecular interactions in the chiral multicomponent crystals and thus decreases the efficiency of the packing, which eventually leads to lower melting points and higher aqueous solubility.